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TECHNICAL REPORT

The Search for New High-Energy-Density Materials

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CONVERSION TABLE

Conversion Factors for U.S. Customary to metric (SI) units of measurement.

MULTIPLY → BY ← DIVIDE
TO GET ← BY → TO GET

angstrom	1.000 000 x E -10	meters (m)
atmosphere (normal)	1.013 25 x E +2	kilo pascal (kPa)
bar	1.000 000 x E +2	kilo pascal (kPa)
barn	1.000 000 x E -28	meter ² (m ²)
British thermal unit (thermochemical)	1.054 350 x E +3	joule (J)
calorie (thermochemical)	4.184 000	joule (J)
cal (thermochemical/cm ²)	4.184 000 x E -2	mega joule/m ² (MJ/m ²)
curie	3.700 000 x E +1	*giga bacquerel (GBq)
degree (angle)	1.745 329 x E -2	radian (rad)
degree Fahrenheit	t _k = (t°f + 459.67)/1.8	degree kelvin (K)
electron volt	1.602 19 x E -19	joule (J)
erg	1.000 000 x E -7	joule (J)
erg/second	1.000 000 x E -7	watt (W)
foot	3.048 000 x E -1	meter (m)
foot-pound-force	1.355 818	joule (J)
gallon (U.S. liquid)	3.785 412 x E -3	meter ³ (m ³)
inch	2.540 000 x E -2	meter (m)
jerk	1.000 000 x E +9	joule (J)
joule/kilogram (J/kg) radiation dose absorbed	1.000 000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448 222 x E +3	newton (N)
kip/inch ² (ksi)	6.894 757 x E +3	kilo pascal (kPa)
ktap	1.000 000 x E +2	newton-second/m ² (N-s/m ²)
micron	1.000 000 x E -6	meter (m)
mil	2.540 000 x E -5	meter (m)
mile (international)	1.609 344 x E +3	meter (m)
ounce	2.834 952 x E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448 222	newton (N)
pound-force inch	1.129 848 x E -1	newton-meter (N-m)
pound-force/inch	1.751 268 x E +2	newton/meter (N/m)
pound-force/foot ²	4.788 026 x E -2	kilo pascal (kPa)
pound-force/inch ² (psi)	6.894 757	kilo pascal (kPa)
pound-mass (lbf avoirdupois)	4.535 924 x E -1	kilogram (kg)
pound-mass-foot ² (moment of inertia)	4.214 011 x E -2	kilogram-meter ² (kg-m ²)
pound-mass/foot ³	1.601 846 x E +1	kilogram-meter ³ (kg/m ³)
rad (radiation dose absorbed)	1.000 000 x E -2	**Gray (Gy)
roentgen	2.579 760 x E -4	coulomb/kilogram (C/kg)
shake	1.000 000 x E -8	second (s)
slug	1.459 390 x E +1	kilogram (kg)
torr (mm Hg, 0° C)	1.333 22 x E -1	kilo pascal (kPa)

*The bacquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (GY) is the SI unit of absorbed radiation.

Objective: The objectives of this DTRA project were to design, by using first-principles density functional theory, new superhalogens capable of involving inner core electrons in chemical bonding, validate the theoretical predictions by carrying out photoelectron spectroscopy experiments, and use thus validated theory to guide experiments in focused discovery of new high energy density materials. Superhalogens belong to a class of highly electronegative species composed of a metal atom at the core surrounded by halogen or oxygen atoms and have electron affinities that are substantially larger than those of the halogen atoms. Early studies on superhalogens involved simple metal atoms such as alkalies, Mg, and Al at the core surrounded by chlorine and fluorine atoms. Our synergistic approach is to involve noble and multivalent transition metal atoms at the core and determine the number of halogens atoms needed to achieve superhalogen behavior. The goal is to enable focused discovery of superhalogen clusters/molecules that can form the building blocks of a novel class of high energy-density salts. We have not only accomplished our goals but also our studies led to a number of discoveries that include a new class of superhalogens that contain neither a metal atom at the core nor halogen atoms on the surface, superhalogens with magnetic properties, and a novel class of electronegative species termed hyperhalogens whose electron affinities are even larger than those of superhalogens. These discoveries have led to a new direction in high energy density materials research and shows promise for synthesizing salts with biocidal properties.

Status of the report: In the first year of the project we completed a comprehensive set of first principles calculations of the structure and stability of CuF_n ($n=1-6$) clusters in neutral and anionic states. We found that all these clusters are stable against dissociation into single F atoms and for $n \geq 2$, the clusters behave like superhalogens.

In the second year we completed several projects. These include a comprehensive study of the structure and stability of XF_n ($X = \text{Cu, Ag, Au}$, $n=1-6$) clusters in neutral and anionic states. We found that all these clusters are stable against dissociation into single F atoms. Neutral XF_4 and anionic XF_5^- clusters are stable against dissociation into F_2 molecules. In addition, anions are more stable than the neutrals suggesting that these clusters can form salts when counter balanced by appropriate positive ions. The fact that coinage metal atoms can bind to as many as six F atoms indicates that their inner $3d$ electrons are participating in chemical bonding. More importantly, the electron affinity of these complexes are as high as 8 eV which is more than a factor of two larger than the electron affinity of the most negative element in the periodic table, namely F (which has an electron affinity of 3.4 eV). Calculations were repeated for CuCl_n clusters. To validate our theoretical procedure photoelectron spectroscopy experiments were carried out on CuCl_n clusters and the results agree with the theoretical prediction.

Studies of FeO_n ($n=1-12$) revealed that clusters with high oxygen content are metastable with no negative frequencies. All of them possess quite high electron affinities and are capable of forming salts with high content of oxygen. Experiments are planned to verify these predictions. We also obtained some unexpected results when reacting Mn atoms with Cl atoms. An entirely new class of highly stable clusters with composition $\text{Mn}_x\text{Cl}_{2x+1}^-$ were discovered whose unusual stability was traced to be due to their

superhalogen properties. In addition, unlike any other superhalogens seen before, these species are magnetic opening the door to the synthesis of a new class of salts with magnetic properties. Unexpected results also were obtained when studying the interaction of Au atoms with oxygen in the pulsed arc ion source insulated with BN. Highly stable clusters consisting of multiple BO_2 ligands were observed. Using density functional theory we traced the origin of these clusters to their superhalogen properties.

Major activities during the third and final year of the project included determining the geometries of metal atoms decorated with electronegative species, studying their stability and spectroscopic properties using first-principles theory and comparing the predictions with photoelectron spectroscopy experiments to validate our theoretical prediction. Theory is then used to search for new negative ions suitable for making salts with biocidal properties. Possible routes to the synthesis of new salts using the superhalogens as building blocks were also suggested. Specific activities included a systematic study of the metal (Al, Sc, Fe) oxide clusters with high content of oxygen, magnetic superhalogens involving Mn and Co as the core atom surrounded by F and Cl, pseudohalogens such as CN as building blocks of a new class of superhalogens with Au atom at the center; BO_2 , BH_4 , and BF_4 superhalogens as building blocks of hyperhalogens with electron affinities much larger than its building blocks; and a novel class of superhalogens that neither contain a metal atom nor halogen atoms. These studies led to many important, yet unexpected results and provided a promising path to synthesize new high energy density materials.

Accomplishments:

We published 26 original articles in some of the most prestigious international journals such as *Angew. Chem. Int. Ed.* where one of the papers was selected as a very important paper (VIP), recognition only 5% of the papers published in this journal receive. The project helped to train a total of 7 postdoctoral fellows and 7 graduate students who received partial support during the tenure of the grant. The PI and Co-PI's gave 83 invited talks at international conferences and seminars at various institutions around the world. In the following we only provide a brief summary of the work performed. Details can be found from the published papers listed in the later part of the report. In the following we briefly describe some of the projects we completed.

Using density functional theory we showed that Cu can indeed have oxidation states ranging from +1 to +4, and possibly +5. Equilibrium geometries of neutral and anionic clusters of CuF_n are shown in Fig.1.

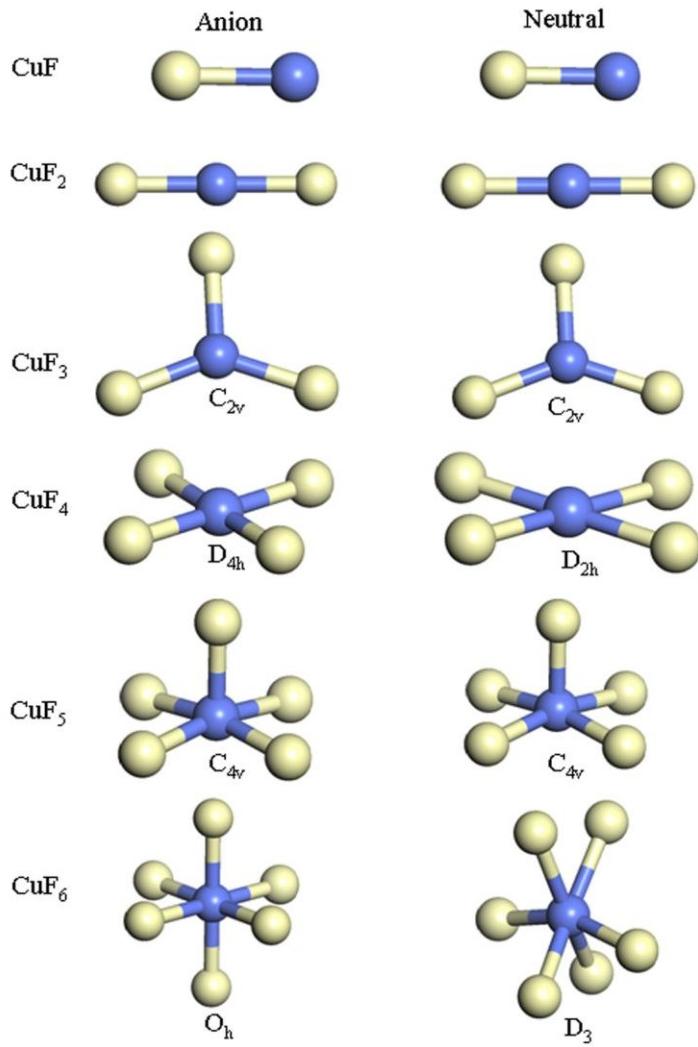


Fig. 1. Optimized geometries of CuF_n neutral and anionic clusters.

Neutral CuF_n clusters are stable in the gas phase against dissociation to F and F_2 for $n \leq 4$ while anion clusters are stable against dissociation to all possible channels for $n \leq 5$ (see Fig. 2).

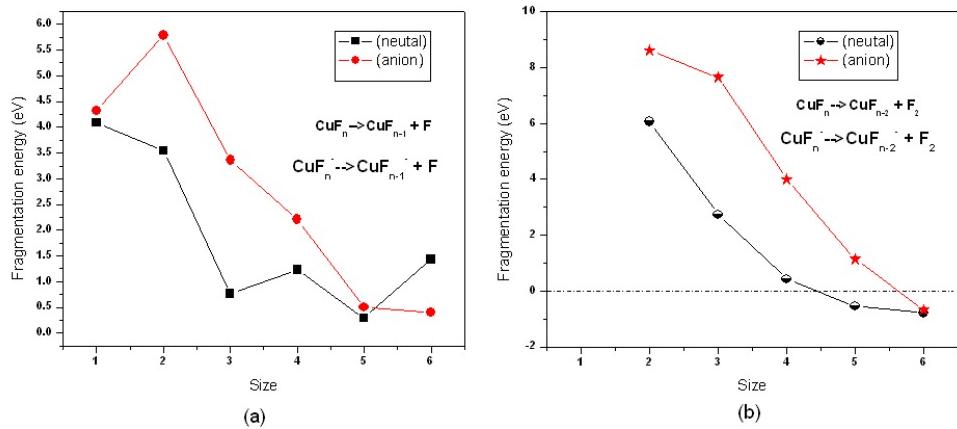


Fig 2. Fragmentation energies for different channels.

The vibrational frequencies of the CuF_6 cluster, both in the anionic and neutral form, are positive which implies that these clusters are at a local minimum and can be stabilized if atomic F is used in their synthesis. The electron affinities of CuF_n clusters increase steadily with n reaching a peak value of 8 eV for CuF_5 . CuF_6 has an electron affinity of 7 eV (see Fig. 3).

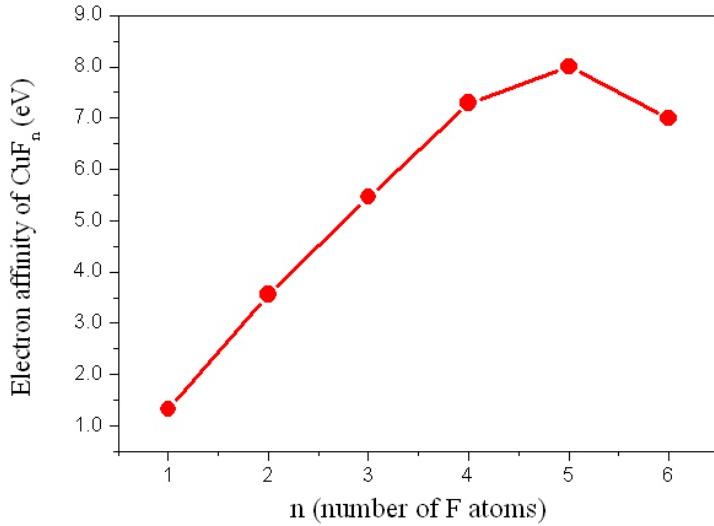


Fig. 3 Electron affinity of CuF_n clusters.

These values are much larger than the electron affinity of F, namely, 3.40 eV. The HOMO-LUMO gaps of these CuF_n clusters range between 1 and 5 eV. For comparison, we note that the HOMO-LUMO gap of C_{60} is only 1.6 eV. Based upon these observations CuF_n clusters can be expected to form the building blocks of a new class of salts with potential applications. We also find that the binding of CuF_n superhalogens to an alkali atom is stronger than that between an alkali atom and F.

To validate our theoretical prediction experiments were carried out at Johns Hopkins University by reacting Cu atoms with atomic chlorine. Note that both Cl and F belong to the same column in the periodic table and have similar chemical properties. In Fig. 4 we show the mass spectra of CuCl_n cluster anions. We note that clusters up to CuCl_6^- exist.

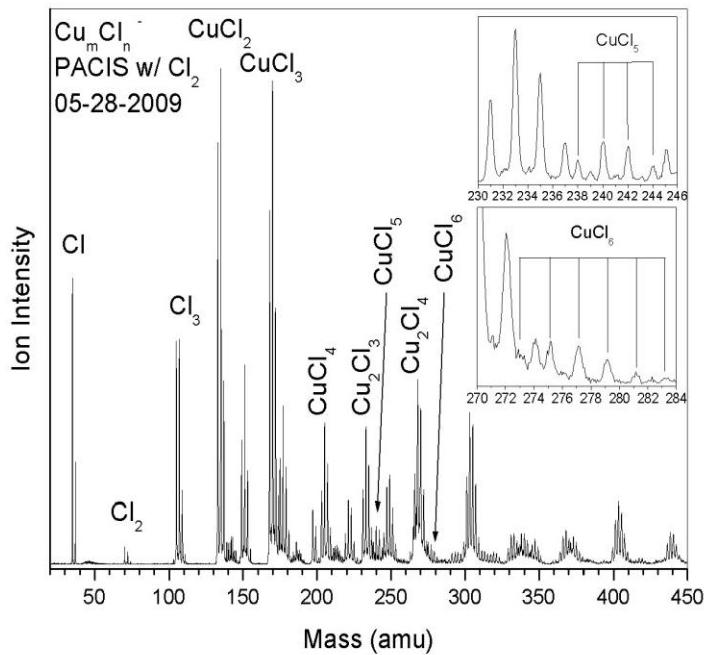


Fig. 4 Mass spectra of CuCl clusters

In particular CuCl₄⁻ did not photodetach with 3.49 eV photons. This implies that the electron affinity of CuCl₄ should be larger than 3.2 eV. This is consistent with our prediction in the CuF_n systems. Experiments are under way to measure the electron affinities of higher CuCl_n clusters by increasing the photon energy.

These results support our original goal of finding transition metal atoms where the involvement of inner *d* core electrons can enable them to bind a large number of halogen atoms. When counterbalanced by positive ions, these negative ions can form salts which can serve as new oxidizing agents.

Using density functional theory we calculated systematically the equilibrium geometries of neutral and anionic clusters of XF_n (X=Cu, Ag, Au, n=1-7) as well as their spectroscopic properties. These results are published as an invited article in Journal of Physical Chemistry. For the purpose of this report we only provide in Fig.5 the electron affinity of the coinage metals as a function of F content. Note that all these clusters containing more than one F atom are superhalogens. That they can bind more F atoms than their nominal valence would permit indicates the involvement of the inner *d* core electrons in chemical bonding.

Electron affinity of coinage metals interacting with flourine

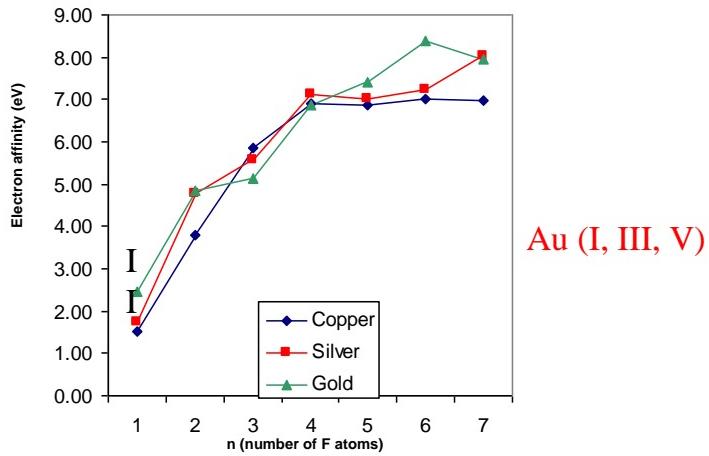


Fig. 5 Electron affinities of coinages metal atoms (Cu, Ag, and Au) interacting with F atoms

Theoretically Predicted EA vs. n for CuCl_n

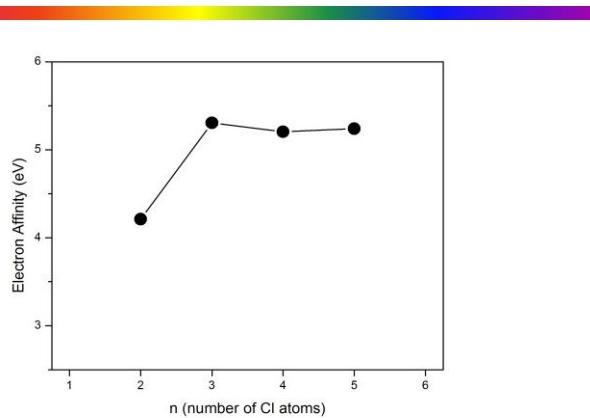


Fig. 6 Theoretically predicted electron affinities of CuCl_n clusters.

To validate our theoretical predictions of the electron affinities (EA), photoelectron spectroscopy studies were carried out by mass selecting Cu_xCl_y clusters produced in a pulsed arc ion source (PACIS). The predicted electron affinities are shown in Fig. 6. The agreement between theory and experimental values of electron affinities are displayed in Figs. 7-9.

Photoelectron spectra of CuCl₂ anion

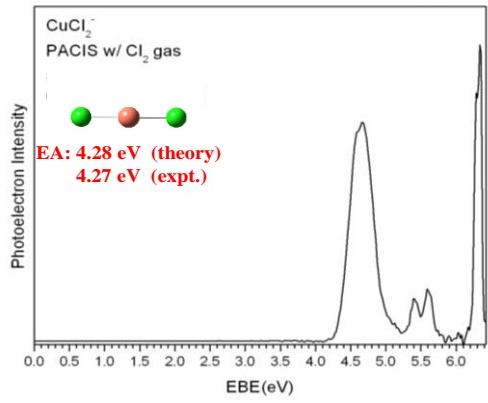


Fig. 7 Computed and measured electron affinities of CuCl₂ cluster.

Photoelectron spectra of CuCl₃ anion

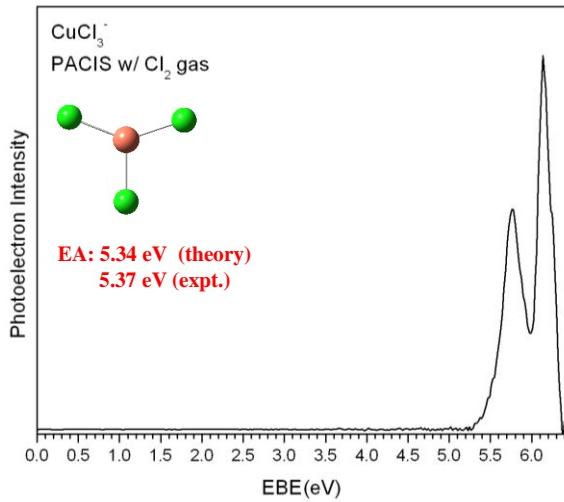


Fig. 8 Computed and measured electron affinities of CuCl₃ cluster.

Photoelectron spectra of Cu₂Cl₄ anion

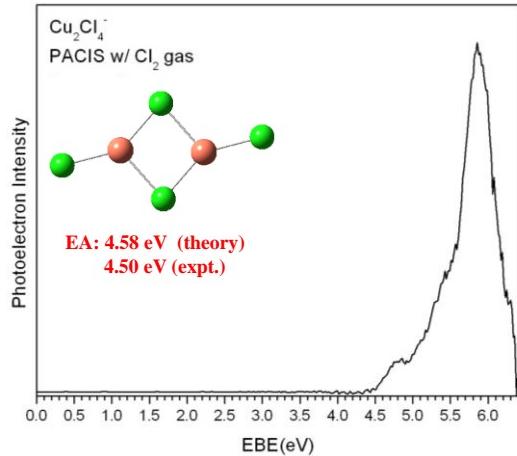


Fig. 9 Computed and measured electron affinities of Cu₂Cl₄ cluster.

The agreement is very good and validates the accuracy of our theoretical approach. In addition, we find that CuCl_y clusters with $y \geq 2$ are superhalogens. Equally important, we also find Cu_xCl_{x+1}clusters are superhalogens where the core is Cu_xCl_x clusters instead of a Cu atom.

DFT calculations were also carried out to see the maximum number of O atoms that can be attached to a single Fe atom. We find that the number of O atoms can be as high as 12 and beyond a critical size, O atoms bind associatively in the peroxy or superoxo form. They also tend to be superhalogens allowing the possibility to produce salts with high oxygen content. In Fig. 10 we show the geometries of some of a neutral FeO₁₂ cluster as an example.

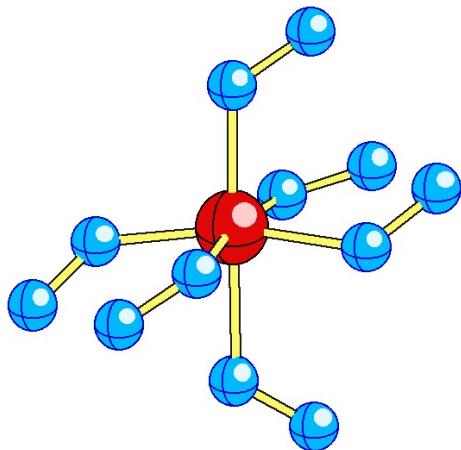


Fig. 10 Equilibrium geometry of FeO₁₂ neutral cluster.

Our studies on superhalogens have enabled us to discover ternary superhalogens that consist of Au atoms surrounded with BO₂ moieties. Note that BO₂, on its own right, is a superhalogen. We hypothesized that an entirely new class of highly electronegative species can be created if halogen atoms are replaced by superhalogen moieties as building blocks. This new class of molecules is expected to have electron affinities higher than its superhalogen building blocks. Using the synergy between theory and experiment we were able to show this to be the case by focusing on Au(BO₂)_x (x=1,2) complexes. This paper published in Ang. Chem. Int. Ed. is classified by the journal as a Very Important Paper (VIP). Only 5% of the articles published in this journal receive this recognition.

The geometrical and electronic structures of Al(BO₂)_n and Al(BO₂)_n⁻ (n = 1–4) clusters are computed at different levels of theory including density functional theory (DFT), hybrid DFT, double-hybrid DFT, and second-order perturbation theory. All aluminum borates are found to be quite stable toward the BO₂ and BO₂ loss in the neutral and anion series, respectively. Al(BO₂)₄ belongs to the class of hyperhalogens composed of smaller superhalogens, and should possess a large adiabatic electron affinity (EA) larger than that of its superhalogen building block BO₂. Indeed, the aluminum tetraborate possesses the EA of 5.6 eV, which, however, is smaller than the EA_{ad} of 7.8 eV of the AlF₄ superhalogen despite the fact that BO₂ is more electronegative than F. The EA decrease in Al(BO₂)₄ is due to the higher thermodynamic stability of Al(BO₂)₄ compared to that of AlF₄. Because of its high EA and thermodynamic stability, Al(BO₂)₄ should be capable of forming salts with electropositive counter ions.

We also discovered a new class of unusually stable clusters with formula Mn_xCl_{2x+1} which are not only superhalogens but also they are magnetic (Fig. 11). This allows the possibility to synthesize a new class of salts with magnetic properties that also can carry a large number of halogen atoms. All the studies thus far have led us to discover superhalogens with super-oxidizing properties and this has been possible only through the synergy between theory and experiment. The last two problems we studied were unexpected and may very well lead to an entirely new way to synthesize salts with novel properties. These results support our original goal of finding transition metal atoms where the involvement of inner *d* core electrons can enable them to bind a large number of halogen atoms. When counterbalanced by positive ions, these negative ions can form salts which can serve as new oxidizing agents.

Mass spectra of Mn_xCl_y clusters

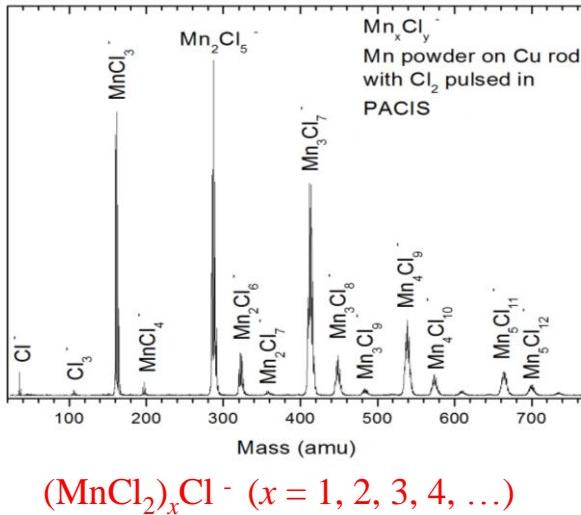


Fig. 11 Mass spectra of Mn_xCl_y anions showing magic peaks with Mn_xCl_{2x+1} composition

Using density functional theory (DFT), we have systematically calculated the equilibrium geometries, electronic structure, and electron detachment energies of $Al(BH_4)_n$ =1- 4 and $Al(BF_4)_n$ ($n=1- 4$) at the B3LYP/6-311+G(2d,p) level of theory. The electron affinities of $Al(BH_4)_n$ not only exhibit odd-even alternation, just as seen in $(BH_4)_n$, but also, for $n = 3$ and 4, show a remarkable behavior: whereas the electron affinities of BH_3 and BH_4 are, respectively, 0.06 and 3.17 eV, those of $Al(BH_4)_3$ and $Al(BH_4)_4$ are 0.71 and 5.56 eV. Results where H is replaced by F are also very different. The electron affinities of BF_3 and BF_4 are, respectively, - 0.44 and +6.86 eV, and those of $Al(BF_4)_3$ and $Al(BF_4)_4$ are 1.82 and 8.86 eV. The results demonstrate not only marked difference when H is replaced by F but also substantially enhanced electron affinities by almost 2 eV when BH_4 and BF_4 units are allowed to decorate a metal atom, confirming the recently observed hyperhalogen behavior of compounds composed of superhalogen building blocks.

We have systematically calculated the ground state geometries, relative stability, electronic structure, and spectroscopic properties of $PtCl_n$ ($n = 1-7$) clusters. The bonding in these clusters is dominated by covalent interaction. In neutral clusters chlorine atoms are chemically bound to Pt up to $n = 5$. However, in neutral $PtCl_6$ and $PtCl_7$ clusters two of the chlorine atoms bind molecularly while the remaining bind as individual atoms. In the negative ions, this happens only in the case of $PtCl_7$ cluster. The geometries of both neutral and anionic clusters can be considered as fragments of an octahedron and are attributed to the stabilization associated with splitting of partially filled d orbitals under the chloride ligand field. The electron affinity of $PtCl_n$ clusters rise steadily with n , reaching a maximum value of 5.81 eV in $PtCl_5$. $PtCl_n$ clusters with $n = 3$ are all

superhalogens with electron affinities larger than that of chlorine. The accuracy of our results has been verified by carrying out photoelectron spectroscopy experiments on PtCl_n^- anion clusters.

We explored the potential of pseudohalogens such as CN, which mimic the chemistry of halogens, to serve as building blocks of new superhalogens. Using calculations based on density functional theory we show that when a central Au atom is surrounded by CN moieties, superhalogens can be created with electron detachment energies as high as 8.4 eV. However, there is a stark contrast between the stability of these superhalogens and that of conventional AuF_n superhalogens. Whereas AuF_n complexes are stable upto n=5 for neutrals and n=6 for anions, $\text{Au}(\text{CN})_n$ complexes (with CN moieties attached individually) are metastable beyond n=1 for neutrals and n=3 for anions. We investigated the nature and origin of these differences. In addition, we elucidate important distinctions between electron affinity (EA) and adiabatic detachment energy (ADE), two terms that are often used synonymously in literature.

The structure, stability, and spectroscopic properties of singly and doubly charged anions composed of simple metal atoms (Na, Mg, Al) decorated with halogens such as Cl and pseudohalogens such as CN were studied. Since pseudohalogens mimic the chemistry of halogen atoms, our objective is to see if pseudohalogens can also form superhalogens much as halogens do and if the critical size for a doubly charged anion depends upon the ligand. The electron affinities of MCl_n ($\text{M}=\text{Na, Mg, Al}$) exceed that of Cl for $n \geq (k+1)$, where k is the normal valence of the metal atom. However, for $\text{M}(\text{CN})_n$ complexes this is only true when $n=k+1$. In addition, while the electron affinities and vertical detachment energies of MCl_n complexes are close to each other, they are markedly different when Cl is replaced by pseudohalogen, CN. The origin of these anomalous results is found to be due to the large binding energy of cyanogen, (NCCN) molecule. Due to the tendency of CN molecules for dimerization, the ground state geometries of the neutral and anionic $\text{M}(\text{CN})_n$ complexes are very different when their number exceed the normal valence of the metal atom. While our calculations support the conclusion of Skurski and coworkers that pseudohalogens can form the building blocks of superhalogens, we show that there is a limitation on the number of CN moieties. Equally important, we find large difference between the ground state geometries of the neutral and anionic $\text{M}(\text{CN})_n$ complexes for $n \geq (k+2)$ which could play an important role in interpreting future experimental data on $\text{M}(\text{CN})_n$ complexes. This is because the electron affinity defined as the energy difference between the ground states of the anion and neutral can be very different from the adiabatic detachment energy defined as the energy difference between the ground state of the anion and its structurally similar neutral isomer.

Using Wade-Mingos rules well known for describing the stability of closo-boranes ($\text{B}_n\text{H}_n^{2-}$) and state of the art theoretical methods we show that a new class of super and hyperhalogens, guided by this rule, can be formed by tailoring the size and composition of borane derivatives. Unlike conventional superhalogens which have a metal atom at the core surrounded by halogen atoms, the superhalogens formed using the Wade-Mingos rule do not have to have either halogen or metal atoms. We demonstrate this by using $\text{B}_{12}\text{H}_{13}$ and its isoelectronic cluster, $\text{CB}_{11}\text{H}_{12}$ as examples. We also show that while

conventional superhalogens containing alkali atoms require at least two halogen atoms, only one borane-like moiety is sufficient to render M(B₁₂H₁₂) (M=Li, Na, K, Rb, Cs) clusters superhalogen properties. In addition, hyperhalogens can be formed by using the above superhalogens as building blocks. Examples include M(B₁₂H₁₃)₂ and M(C-B₁₁H₁₂)₂ (M=Li - Cs). This finding opens the door to an untapped source of superhalogens and weakly coordinating anions with potential applications.

Our work is supporting the DTRA mission in advancing fundamental understanding of how physics and chemistry can be manipulated at the nanoscale to design materials for applications as high energy-density materials. In particular, a systematic pathway for discovering a new class of superhalogens is under way. When balanced by counter positively-charged ions, these anions can constitute a new class of salts that can carry a large amount of F safely. The project is also helping to educate students and postdoctoral fellows in state-of-the-art modeling and experimentation, and increase the pool of minorities and women in science.

Personnel Supported:

Virginia Commonwealth University

P. I., Puru Jena (5/25/11 - 8/09/11)

Postdoctoral fellows

Anil Kandalam (6/10/09-6/24/09; 5/25/11-7/24/11),
Qian Wang (6/10/09-12/09/09; 1/10/12-3/09/12),
Qiang Sun (1/10/12-3/09/12),
Bikash Gupta (1/10/12-3/09/12),
Kalpataru Pradhan (10/24/09-10/09/11),
Sa Li (2/25/10-5/09/11).

Graduate Students:

Miaomiao Wu (10/10/09-10/09/11)

Johns Hopkins University

Co-P.I. Kit Bowen (1 mo. supplemental salary/per yr)

Graduate Students:

Angela Buonaugurio, 15 months
Di Wang, 8 months
Haopeng Wang, 7 months
Jacob Graham, 3 months
Xinxing Zhang, 3 months
Allyson Buytendyk, 3 months

Florida A&M University

Gennady Gutsev (senior research scientist)

Publications:

Sun, Q., Wang, Q., and Jena, P.: “Superhalogen properties of CuF_n clusters”, *J. Chem. Phys.* **131**, 124301 (2009).

Gotz, M., Willis, M., Kandalam, A., Gantefor, G. G., Jena, P.: “Origin of the unusual properties of Au_n(BO₂) Clusters”, *Chem. Phys. Chem.* **11**, 853 (2010).

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Interactions/Transitions:

a. Participation/presentation at meetings, conferences, seminars

Invited talks at conferences

P. Jena (P.I.)

Workshop on High Energy Density Materials, Indian Head, MD, May 7, 2009

Power and Energy Workshop, Valparaiso, Chile, June 30-July 1, 2009

Commonwealth NanoScience Workshop, Charlottesville, VA, July 27, 2009

American Chemical Society, Washington DC, August 16-20, 2009

5th Conference of the ACCMS, Hanoi (key note), Vietnam, September 7-11, 2009

European School on Computational Nanoscience for Renewable Energy Systems, Helsinki, Finland, September 13-18, 2009

Computational materials science network workshop on "Predictive Modeling of the Growth and Properties of Energy-Relevant Thin Films and Nanostructures", Denver, Colorado, October 18-20, 2009

The 2nd Annual International Conference on Energy, Logistics and the Environment", Las Vegas, Nevada, Oct. 22-24, 2009

Asian Consortium Condensed Matter Sciences Workshop, Sendai, Japan, January 12-14, 2010.

Materials Challenges in Alternative & Renewable Energy, American Ceramic Society, Cocoa Beach, FL, February 21-25, 2010

US-Egypt Advanced Studies Institute (ASI) on "Nanomaterials and Nanocatalysis for Energy, Petrochemicals and Environmental Applications", Cairo, Egypt, March 27 – April 5, 2010

U.S.-Russia Experts Meeting on Nanoscience for Energy, Department of State, Washington, D.C., April 8-9, 2010

2010 Workshop of the International Centre for Quantum Structures (ICQS), Beijing and Xiamen, China, June 7-11, 2010,

12th International Conference on Modern Materials and Technologies – (5th Forum on New Materials) Montecatini Terme, Tuscany, Italy, June 13- 18, 2010

Gordon Research Conference on Energetic Materials, Tilton School in Tilton, NH, 13 – 18 June 2010.

Cluster-Surface Interactions Workshop, Stratford-upon-Avon, UK, July 5-8, 2010

International Workshop on “Simulations and Experiments on Materials for Hydrogen Storage”, Dublin October 11-13, 2010

Current Trends in Condensed Matter Physics Workshop, Bhubaneswar, India, December 15-19, 2010

Academy of Finland Centre of Excellence Program – The Expert Panel on 9 and 10 February 2011

Presidential Commission on USA-Russia Cooperation on Nanoscience for Energy, Moscow, February 28-March 4, 2011

DOE-BES Contractors’ meeting “Physical Behavior of Materials, Airlie Center, Virginia March 6-9, 2011

International School and Symposium on Multifunctional Molecule-based Materials, Argonne National Laboratory, March 13-18, 2011

Study of Matter at Extreme Conditions - SMEC 2011 Conference, Miami, Florida, Materials under Extreme Conditions, Miami, March 27-April 2, 2011

Size selected and supported clusters, Davos, Switzerland, March 20-25, 2011

Collaborative Conference on 3D & Materials Research (3DMR), Ramada Plaza Hotel at the Jeju Island, South Korea, June 27 - July 1, 2011

Asian Consortium on Condensed Matter Sciences Workshop, Singapore, September 6-9, 2011

India Science Exhibition, Khoj, Mumbai, India, October 1-2, 2011

South Eastern Regional Meeting of the ACS, Richmond, VA, October 26-29, 2011

Quimi UNAM 2011, Mexico City, Mexico, 2011

International workshop on Functional Materials, Berhampur, Orissa, India December 20-22, 2011

GRI Symposium III on Cluster Science, Nagoya, Japan, February 1-3, 2012

Materials in Renewable Energy, Clearwater, Florida, February 26 – March 1, 2012

Materials genome: Simulation, Synthesis, Characterization, Manufacturing, April 4-6, Terranea Resort, CA 2012

Kit Bowen (Co PI) (Invited talks related to this project, about 30 during the project period)

DTRA Program Review, Arlington, October 26-28, 2009

DTRA Program Review, Arlington, May 25-27, 2010

DTRA Program Review, Arlington, July 27, 2011

Gordon Conference on High Energy Density Materials, Dover, Vermont, June 17-22, 2012

Invited Seminars

P. Jena (P.I.)

Foreign Service Institute, Arlington, VA, June 17, 2009

University of Tennessee, Knoxville, October 1, 2009

Mc Neese State University, Lake Charles, LA, November 18, 2009

University of Tennessee, Knoxville, TN, May 6, 2010

Oak Ridge National Laboratory, Distinguished Lecture, May 7, 2010

Foreign Service Institute, Arlington, VA, June 23, 2010

Peking University, Beijing, China, June 8, 2010

Institute of Solid State Physics, Heifei, China, June 9, 2010

Florida International Univ., Miami, Florida, November 19, 2010

University of Uppsala, Uppsala, Sweden, December 10, 2010

S. N. Bose National Instutute, Kolkata, India, December 18, 2010

EMPA, Dubendorf, Switzerland, March 26, 2011

Johns Hopkins University, Baltimore, Maryland, April 18, 2011

Foreign Service Institute, Arlington, June 22, 2011,

Reliance Corporation, Mumbai, India, October 3, 2011

Indian Institute of Technology, Mumbai, India, October 4, 2011

University of Hyderabad, Hyderabad, India, October 6, 2011

Jawaharlal Nehru University, New Delhi, India, October 8, 2011

University of Tennessee, Knoxville, Tennessee, April 2, 2012

b. *Consultative and advisory functions*

The P.I. in his capacity as a Jefferson Science Fellow regularly consults with the State Department on matters related to science and diplomacy.

c. *Transitions*

Knowledge resulting from this work will be used to synthesize a new class of salts containing superhalogen clusters as building blocks.

New discoveries, inventions, or patent disclosures:

An invention disclosure has been filed by Virginia Commonwealth University on hyperhalogens.

Honors/Awards:

Life time achievement honors of P. Jena (P. I.)

- Presidential Medallion, Virginia Commonwealth University, 2011
- Jefferson Science Fellow, US Department of State, 2007-08
- Outstanding Faculty Award, State Council of Higher Education of Virginia (the highest honor given by the Commonwealth of Virginia), 2001
- Fellow, American Physical Society, 2000
- University Award of Excellence, Virginia Commonwealth University (the highest honor given by Virginia Commonwealth University), 1993
- Distinguished Scholar Award, Virginia Commonwealth University, 1987

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